Committee Report
NSLS-II Experimental Facilities Advisory Committee Meeting
October 4-5, 2007

Members Present:

A. Baron, SPring8
M. Chance, Case Western Reserve University
Jerry Hastings, SLAC
Gene Ice, ORNL
Andrzej Joachimiak, ANL
Steve Kevan, University of Oregon
Robert Lieberman, Stony Brook University
Simon Mochrie, Yale University, Chair
Mohan Ramanathan, ANL
Ian Robinson, University College, London
Francesco Sette, ESRF
Brian Stephenson, ANL

Members Absent:

P. Dumas, SOLEIL

The NSLS-II EFAC met on October 4 and 5, 2007 and heard presentations providing an overview of the current project status, including detailed plans for experimental stations on 6 insertion devices, that are envisioned as part of the NSLS-II project. These include a soft x-ray coherent beamline, a coherent hard x-ray diffraction imaging (CXDI) station, an x-ray photon correlation spectroscopy/small-angle-x-ray-scattering (XPCS/SAXS) station, a nanoprobe station, a 0.1 meV-resolution inelastic x-ray scattering (IXS) station, a high-energy powder diffraction station, and an XAS station.

The EFAC compliments the NSLS-II staff not only for their lucid presentations, but also for the tremendous amount of work that each presentation represents. The suite of beamlines described will unquestionably address a number of cutting-edge scientific questions, encompassing the key scientific goals of the NSLS-II facility. In addition, the mix of beamlines presented will serve to preserve and promote the broad interests of the current NSLS scientific community, as well as attract new users to NSLS-II.

The beamline designs were presented in sufficient detail to convince the EFAC that such a suite of beamlines can be designed, constructed, and commissioned within the stated cost envelope, which is consistent with the costs of other recent and ongoing beamline construction projects. We judge too that the schedule is realistic based on the anticipated ramp-up in staffing. Overall, the EFAC is very favorably impressed with the management aspects of the NSLS-II project. We particularly appreciate the new “Issues Tracking” system as applied to EFAC comments/issues.

NSLS-II has the capacity for on the order of 60 beamlines, and needs to develop, in concert with its users, a cohesive, facility-wide plan that both exploits the unique capabilities of the NSLS-II source and accommodates the large and productive existing NSLS user community. Beamline development within the NSLS-II project will provide a minimum suite of insertion device beamlines for BES-relevant science to ensure that an appropriate minimal set of capabilities is present at the outset. In this regard, it is essential at this stage that the project preserve sufficient flexibility in the definition of the suite of project beamlines, so that community input via the imminent Letter of Interest (LOI) process can be properly incorporated, consistent with the twin goals of both exploiting the unique capabilities of the NSLS-II source and accommodating the large existing NSLS user community.

The EFAC heard an outline proposal for the beamline development process, namely that all beamlines are to be developed based on community input via so-called Beamline Advisory Teams (BATs). The BATs are small teams, formed to represent a particular user community. Their initial role is to develop a scientific mission and the corresponding technical requirements for each beamline. The EFAC endorses this definition of BATs, as representatives of a user community. Each BAT will submit a “Letter of Interest” (LOI) for the beamline in question, which will then be reviewed by the EFAC. (We feel that “Letter of Interest” is a more appropriate name than “Letter of Intent”.) Once approved and funded, it is anticipated that NSLS-II will then staff, design, and construct the beamline. The EFAC generally endorses this model, although we encourage NSLS-II management to carefully examine in an ongoing fashion and on a case-by-case basis whether and how macromolecular crystallography (MX) beamlines in particular, and life-sciences beamlines in general, as well as other non-BES-funded beamlines will best be implemented within this context. In the case of BES-funded beamlines, the continuing role of the BAT, beyond the LOI stage, is to offer detailed advice to the beamline staff, during design, construction, commissioning, and early operations, reporting to the Experimental Facilities Division (XFD) Director. In the non-BES-funded case, the BATs will play an essential additional role in raising funds for beamline design, construction, and commissioning. We encourage NSLS-II to remain open to the possibility that these BATs may transition into teams that raise funds for, and participate in, beamline operations as well.

The EFAC also endorses the advisory role envisioned for the BATs and commends NSLS-II for clarity in relation to the fact that there will be no preferential access to BAT members beyond the beamline-commissioning phase. It is important to ensure that this is clearly communicated to the wide user community

The EFAC endorses the process outlined above for all types of beamlines, including the project beamlines, beamlines funded as Major Items of Equipment (MIEs), beamlines funded from non-BES sources, and beamlines transferred from NSLS. We furthermore endorse the proposed content of the LOIs, namely that they should specify the scientific case for the beamline, the technical requirements of the beamline, including the required source, how the proposed beamline meets the needs of the user community, and the expertise of the BAT members.

We also endorse the proposed criteria for beamline selection, namely excellence of the scientific case and engagement of the user community in its articulation, best-in-class beamline performance with characteristics well matched to NSLS-II source, technical feasibility of reaching the beamline's scientific objectives, alignment with an overall sensible utilization of the facility, and the quality of the BAT.

We also endorse the schedule for an open call for LOIs of all types, including those leading to complete beamlines, as well as less-well-defined LOIs for contributions to scientific cases or proposed instrumentation. In view of the broad expertise within the EFAC, we anticipate that, in most cases, two expert EFAC members will be assigned to focus on each LOI. Their work will then form the basis for deliberations by the entire EFAC. If circumstances warrant, external experts may also be consulted.

At each round of reviews, the EFAC requests that we be provided with the NSLS-II's overall vision for what a fully built-out NSLS-II will look like. It is to be expected that this vision may evolve in time in response to user input, as expressed via the BAT process itself. However, being able to carry out reviews in the context of such an overall plan will permit the EFAC to ensure that EFAC-approved beamlines indeed correspond to an overall sensible mix for NSLS-II, as it evolves.

The EFAC applauds the successful hiring of a number of outstanding new staff, especially beamline staff, to the NSLS-II project. Nevertheless, personnel and staffing remains a critical issue for NSLS-II, and there is an urgent need to hire additional people to complement the current outstanding staff. This is a particularly important issue in view of the facts, first, that it is anticipated that the first proposal for "Major Items of Equipment" beamlines will be submitted in Spring/Summer 2008, and, second, that in order to ensure continuity for the large life science community currently carrying out research at the NSLS, it is the EFAC's strong recommendation that NSLS-II plan to make one or more life sciences beamlines operational on a similar schedule to the project beamlines; that is, there should be operational life sciences beamlines right from the start of NSLS-II operations. The EFAC applauds the detailed coordination between NSLS and NSLS-II that is on-going with respect to staff and urges that such close cooperation continue. We also encourage the appointment of an NSLS-II Deputy Director for Life Sciences, who will take a lead in developing a strategic plan for the life sciences in concert with users.

It is critical for staff recruitment and retention that there should be opportunities for career growth and development. Therefore, beamline staff should be encouraged to initiate and develop their own research programs. Of course, this may be in collaboration with scientists outside NSLS-II, for example, in the context of JPSI, but it need not be. The EFAC wholeheartedly supports that the predominant mode of user access on all beamlines will be through peer-reviewed proposals, typically using the GU program of the facility. However, to facilitate staff research, and ensure that there are ongoing developments to maintain each beamline at the scientific forefront, the EFAC urges that 10% of the beamtime at NSLS-II be allocated for beamline staff research. This time should not preclude the beamline staff from submitting General User (GU) proposals.

However, such an allocation is essential to ensure that the facility become as scientifically productive as possible. Specifically, instead of the desirable collaborative relationship that should exist between beamline staff and GUs, in the absence of such an allocation, beamline scientists are placed in direct competition with GUs for all of their – the beamline scientist's -- beamtime. The result would be a major disincentive for beamline scientists to make beamlines user-friendly, and to recruit new GUs and programs to NSLS-II, and to work with existing GUs to improve and refine the GUs' proposals and experiments. The EFAC notes, moreover, that such an allocation is entirely in-line with what occurs at other synchrotrons.

The EFAC was pleased with the plan to develop a robust effort in the area of coherent soft x-ray (CSX) science. The capabilities of the proposed beamline and end stations are well conceived and provide a good starting point for continued planning and design. There is a strong nucleus staff shepherding this project. We have several specific comments concerning this part of the NSLS-II project.

While the planned CSX scientific program was not discussed in detail, the current conceptual beamline design will serve the needs of many different experiments. The NSLS-II will be a unique source, and applications of coherent soft x-ray beams occupy a high-risk niche. The facility has started to engage the user community with workshops designed to focus on a few high profile applications that clearly leverage this combination of uniqueness and risk. This process should continue so the facility can focus its resources toward achieving those goals.

We support the plan to implement low- and high-resolution monochromators that share a single set of chicaned undulators, as this will enable a useful trade-off between coherent flux and energy resolution. We were surprised that there was no mention of inelastic soft x-ray scattering in the experimental portfolio. The high-resolution beamline will position the NSLS-II to accomplish seminally important measurements of the low energy excitations, for example, in complex oxides and magnetic systems. Such measurements will complement the hard x-ray inelastic scattering program. Similarly, we were surprised that there was no mention of a high field capability in the end stations. An important goal of nanoscience is to measure and control complexity with non-themal parameters, and in the context of the capabilities of this proposed beamline, to apply high magnetic field will clearly be very important.

Polarization switching using kicker magnets in the coherent soft x-ray sector requires detailed study to ensure that this will not adversely impact performance of other beamlines. This capability is only incrementally better than polarization switching using beamline optics, and the many trade-offs need to be carefully considered.

We strongly endorse the 0.1 meV inelastic x-ray scattering (IXS) program as moving the established and highly successful IXS technique into a new and unmatched regime. This should be immediately useful for investigating the crossover between continuum and short wavelength dynamics in disordered materials, and is expected to find other uses with increased experience, as it will be the first spectrometer of its kind. To aid in defining the effort, and to highlight the tradeoffs involved in design choices, we encourage NSLS-II to develop a plan (or plans) for first experiment(s). Specific considerations should include (1) the competition between the amount of focusing needed for spectrometer operation and the desired momentum resolution (2) the required analyzer angular acceptance and (3) the momentum space range of the instrument. We expect rough count-rate estimates can also be extrapolated from present-day experiments.

The 0.1 meV spectrometer will need an extremely high-flux and high-brilliance insertion device, requiring that this beamline be one of the most powerful at NSLS-II at its ~ 9 keV operational energy. At the same time, the 0.1 meV instrument is experimental, with components beyond the present state of the art. This very challenging endeavor may require intermediate steps before achieving the ultimate 0.1 meV resolution. However, operation at resolution below 1 meV is already attractive for new science, especially in consideration of the resolution function for the new spectrometer, which is expected to be much sharper than that of present-day backscattering spectrometers. Effort should be made to foster user-community interest in the 0.1 meV instrument.

In view of the extremely powerful insertion device needed for the 0.1 meV spectrometer, the beyond-state-of-the-art nature of the required instrumentation, and the long outstanding tradition of NSLS in developing and using IXS to investigate electronic excitations, we suggest that a 50 meV spectrometer for electronic excitations be considered at the same beamline as the 0.1 meV spectrometer. A state-of-the-art 50 meV spectrometer is extremely well matched to the available energy range, and will strongly benefit from BNL in-house expertise in area detectors. In our opinion, it is better matched to the planned beamline than the separate ~meV backscattering spectrometer considered previously: the technology to make ~meV resolution backscattering at 9 keV remains unproven, while successful meV instruments, operating near 22 keV, exist at all high-energy third generation storage rings, including the APS. Importantly, a 50 meV instrument also addresses the needs of an established user community, which will not have access to such an instrument at other third generation sources in the foreseeable future. Therefore, we suggest a 50 meV spectrometer should be constructed on the 0.1 meV beamline, to be available at the early stage of operation of the NSLS-II.

The Hard Coherent X-Ray Beamline will realize a number of unique cutting-edge scientific opportunities. For example, the ability to image crystalline particles down to 10nm diameter will revolutionise our knowledge of how catalyst particles change shape as they function. The application of CXDI to image strains within nanoscale semiconductor devices will lead to entirely new technologies. The XPCS method and related SAXS capabilities will have a transformative impact on our understanding of the structure and dynamics of soft and disordered matter. The use of a long beamline and customised XPCS detector combined with the significantly higher brightness of NSLS-II compared to other sources will allow these techniques to go far beyond any competition. However, the EFAC notes the recommendations of last month’s Comprehensive Design Review that separating the hard x-ray XPCS and coherent diffraction beamlines by putting them on different undulator ports will give each of them full independence. Separating CXDI and XPCS will also eliminate the obstacle of having a transport pipe in close proximity to the XPCS sample position, and the requirement that the two experiments run at the same energy. Such a strategy will moreover facilitate possible future upgrades, for example, to add a second undulator for XPCS, which is a brightness limited technique. The scientific impact of these two programs is very significant, which may warrant the additional cost of dedicating an extra port and the additional financial burden of undulator, front end and FOE.

The Nanoprobe Station will take advantage of the very high brightness of NSLS-II to allow x-ray imaging at unprecedented resolution. The EFAC has confidence that the beamline design will support state-of-the-art x-ray microscopy during the life of NSLS-II by delivering the full coherent flux to the endstation. The optical design is similar to that recently constructed at APS Sector 26. The overall cost estimate and schedule plan are consistent with that project, and the similarity in design gives high confidence in the estimates for setting the project baseline.

Regarding the nanoprobe instrument, continuing developments in x-ray microscope technology (e.g. by XRADIA, at SSRL, and at beamlines worldwide) will likely make the goal of better than 1 nm positioning accuracy achievable. Resolutions of < 0.01 nm in a single axis have already been demonstrated in the laboratory. Nanofocusing x-ray optics development will be key to achieving the 1 nm imaging resolution goal, which is well beyond current state of the art. The EFAC strongly supports the proposed R&D program for nanofocusing optics development in parallel with beamline design and construction. This will ensure that world-leading capabilities are available at the beginning of operations, and form the basis for a continuing research program at NSLS-II to keep the facility at the forefront in x-ray nanofocusing.

The current machine and undulator parameters, which produce a gap in the available energy range in the 4-5 keV region, will however compromise the ability to perform spectromicroscopy at the K edges of elements such as Ca, Sc, and Ti, and at L edges of elements in the range 48-55. We encourage the development of a long-term strategy to cover this energy range at the Nanoprobe Station, such as adding a second undulator with different spectral output. We would like too to better understand the trade-offs required to possibly future 3.6 GeV operations.

X-ray Absorption Spectroscopy is a popular technique used extensively for various disciplines such as materials, environmental and life sciences. The NSLS presently has a large user community using XAS techniques among the various beamlines. Experimental facilities staff at NSLS-II has to be commended on having organized numerous workshops and having sought input from various user communities to bring forward plans for a proposed XAS beamline at NSLS-II. The plan to use the damping wiggler is a good choice for the XAS program, as it provides a clean spectrum over a large energy range. There is significant flux even at 90 keV from the damping wiggler source. There are numerous challenges in beamline optics due to immense power load from the damping wiggler. NSLS-II staff has presented realistic plans to handle the power and much R&D is expected in this area.

With regard to the proposed powder diffraction beamline, we note that the study of condensed matter at extreme conditions is developing into a very rich field. *In situ* elastic scattering provides the data required to derive structure models, which is essential to systematic searches for new classes of materials and to rationalizing their desirable properties. The proposed powder diffractometer at NSLS-II will be the US' only high-resolution instrument capable of collecting data at high energies (> 50 keV). This will make it ideal for *in situ* and time-resolved studies of samples held in environmental cells [e.g. the high-pressure diamond-anvil cells or the larger-volume Paris-Edinburgh cells]. Current practice at beamlines at APS are hamstrung by lack of energy discrimination of the detectors used, and contamination of the X-ray elastic scattering signal by parasitic scattering from cell components. Tight collimation effectively discriminates against parasitic scattering amd the higher energies will make this new beamline ideal for studies using the atomic pair distribution function [PDF] method. The new instrument will allow enhancement of the elastic signal, including the diffuse component required to evaluate technologically important disordered condensed matter, by employing the crystal analyzer array. This will provide the highest possible signal-to-noise discrimination and the evaluation of lower Z-containing materials (ice clathrates for example), ferritin cores and a host of other interesting materials.

The presentation of plans for this beamline included some important scientific thrusts for the total high-energy X-ray elastic scattering [THEXES. However, it is important that the dialogue between the beamline technical design team and the scientific user community continue and be vigorously pursued so that the optimum beamline is designed and constructed to serve the most important scientific thrusts as well as the broadest and deepest user community.

Although life sciences beamlines are not part of the NSLS-II construction project, nevertheless, it is clear that biology will constitute a large and essential component of future NSLS-II research. Thus, it is imperative that the planning and funding for this effort should be organized in parallel with the project timeline. In consideration of the challenges involved, at its May 2007 meeting the EFAC recommended the appointment of a individual with responsibility for coordination of strategic planning for life sciences within the context of NSLS-II, in particular, focusing on the scientific scope for biology programs at the NSLS-II, interacting with users, and with the funding agencies. The EFAC commends NSLS-II management for moving forward on this recommendation and we urge the hiring of an NSLS-II Deputy Director for Life Sciences as soon as possible.

The EFAC expects that the NSLS-II biology capabilities will include an integrated suite of state-of-the-art biology beamlines with a wide range of advanced capabilities serving both regional and national user communities. These likely will include: (1) macromolecular crystallography with advanced robotic capabilities for high-throughput structure determination and able as well to address the most challenging structural biology problems, and studies of nano-biomaterials; (2) high-resolution structural and chemical imaging of biological systems; (3) other high-resolution structural molecular biology techniques such as X-ray absorption spectroscopy, x-ray footprinting, small angle x-ray scattering, infrared and other relevant approaches.

The above scientific priorities encompass efforts both to take advantage of unique capabilities of the NSLS-II and to promote and preserve existing and emerging life science user communities. In order for these user communities to thrive within the NSLS-II project plan it is essential that state-of-the art insertion device beamline capabilities be available for Life Science experiments at the same time that the NSLS-II project beamlines come up. This will require the Life Sciences user community to coordinate a vision for Life Sciences at the NSLS-II, raise significant funds from agencies such as NIH, NSF, and DOE (OBER), and begin their design and construction activities very soon. The NSLS-II should support these efforts, as well as consider collaborative mechanisms that will encourage and facilitate the participation of the user community in the large effort that will be required to achieve these goals.

The EFAC also heard the current plans for moving existing research programs and moving and possibly upgrading existing beamlines from NSLS to NSLS-II. We support the proposed use of LOIs to initiate this process followed by EFAC review. The transition plan needs to be carefully monitored in an ongoing fashion, especially with regard to timeline and staffing issues, to minimize any interruption of the various user programs. It is critical that the process be carried out to assure minimal impact on user science during the transition. In this regard, the EFAC strongly recommends that there occur a minimum of 1 year of overlap of NSLS operations and NSLS-II user operations in order to preserve and promote the NSLS/NSLS-II user community.

The EFAC was pleased to hear about BNL’s proposal for an advanced detector development program, and urges the DOE to fully fund it. For many experiments, an improved x-ray detector would yield a far greater improvement in experimental throughput or precision than anything else. Now is an opportune time to initiate such a program at BNL, in particular, in and in the US more generally. Recently, a number of European detectors efforts – such as Pilatus and Medepix -- are starting to bear fruit, although none of them approach the revolutionary vision, for example, to create a detector that will revolutionize XPCS, that was laid out by Peter Siddons. In particular, for XPCS experiments, the detector is THE critical aspect. In order to characterize processes occurring on microsecond time scales, it is necessary to have a detector that has a time resolution of 1 microsecond or better, that has many pixels, and has near unity quantum efficiency for x-ray detection. This is far beyond the capabilities of all presently available x-ray area detectors.